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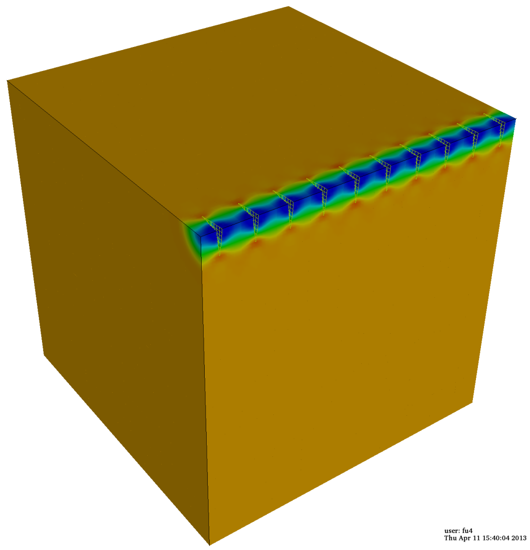

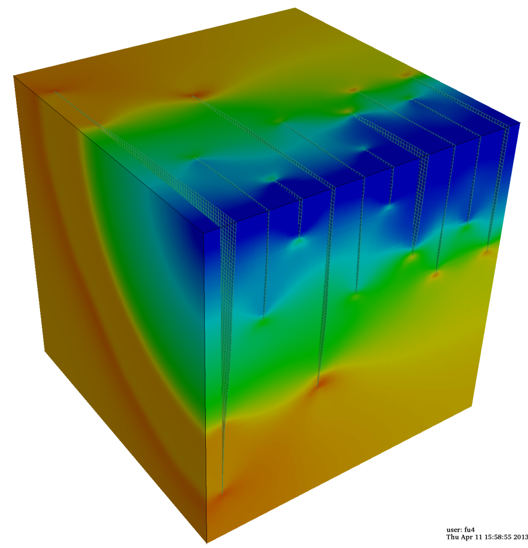

GEOS Code Development Road Map

Scott Johnson, Randolph Settgast, Pengcheng Fu, Tarabay Antoun and F.J. Ryerson

GEOS is a massively parallel computational framework designed to enable HPC-based simulations of subsurface reservoir stimulation activities with the goal of optimizing current operations and evaluating innovative stimulation methods. GEOS will enable coupling of different solvers associated with the various physical processes occurring during reservoir stimulation in unique and sophisticated ways, adapted to various geologic settings, materials and stimulation methods. The overall architecture of the framework includes consistent data structures and will allow incorporation of additional physical and materials models as demanded by future applications. Along with predicting the initiation, propagation and reactivation of fractures, GEOS will also generate a seismic source term that can be linked with seismic wave propagation codes to generate synthetic microseismicity at surface and downhole arrays. Similarly, the output from GEOS can be linked with existing fluid/thermal transport codes. GEOS can also be linked with existing, non-intrusive uncertainty quantification schemes to constrain uncertainty in its predictions and sensitivity to the various parameters describing the reservoir and stimulation operations. We anticipate that an implicit-explicit 3D version of GEOS, including a preliminary seismic source model, will be available for parametric testing and validation against experimental and field data by Oct. 1, 2013.

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On the cover**. **GEOS 3D simulation of fracture propagation along a horizontal well. We used a constant boundary condition at the center of each fracture and variations in pumping pressure of less than 0.5%. Running in explicit mode, the simulation used 960 processors and took 15 hours. For the solid body, blue represents compression, red tension. For the fluid, red represents higher fluid pressure.

1. *GEOS* - A massively-parallel simulation framework

Due to the vast range of relevant time and spatial domains, coupled with uncertain boundary conditions, the development of numerical simulation tools to address problems in the geological sciences and geologic engineering applications represents a continuing challenge. It has been difficult to develop effective numerical tools that incorporate accurate models of the relevant physical mechanisms and the requisite spatial and temporal scaling, while maintaining computational economy. Instead, many tools have been developed utilizing field-based experience and/or empirical relationships, and can work extraordinarily well when the operation is mature and a significant operational database exists. These methods, however, work less well when one needs to predict the outcome of a new operational method or work in a reservoir that has geologic characteristics different from those that are familiar. Such complexities are encountered in unconventional gas and oil production, development of enhanced geothermal systems and in geologic carbon sequestration – each an important energy security and environmental concern. However, it is these new operational methods and unfamiliar geologies that hold the greatest prospect for unlocking new energy resources and increasing the efficiency of resources extraction.

Currently, the oil and gas industry has been able to address hydraulic stimulation operations from a largely empirical standpoint. The advent of slickwater hydraulic fracture stimulation, coupled with horizontal drilling and staged fracturing, the technologies that have spurred the current boom in tight gas drilling, is an example of such an advance. This is emblematic of many advances, where trial-and-error over many projects by many operators eventually results in a technique that works and has generated both wealth and major new domestic reserves. Unfortunately, this empirical approach can be inefficient in terms of resource allocation (the cost of drilling a single well can be ~$1M) and may also have significant environmental costs and consequences. This approach also has raised concerns about total recovery efficiency, and if current practice will prevent future recovery of reserves. Finally, through learning and application industry has identified many uncertainties and likely inefficiencies that would benefit from advanced approaches especially advanced simulation and modeiing.

The primary issue addressed by the ***GEOS Initiative*** is whether or not advanced simulation can help to optimize existing extraction operations, to reduce drilling and lifing costs, to evaluate the efficacy of innovative methodologies, and dramatically improve environmental stewardship. It is our experience and expectation that at this stage, many of those solutions high performance computing (HPC) applied to a range of geologic models informed and validated by field data from commercial production sites and operations. Given the ever-increasing need for energy with minimal environmental impact, the prospects of simulation in optimizing operations, during both planning and execution, is tantalizing.

The major hurdle in developing such numerical simulation tools lies in two domains: the complex physical processes at work in the reservoir, and the uncertain nature of reservoir characteristics. Processes associated with stimulation vary drastically in time and spatial extent, and the dominant physical processes at any location within a reservoir may also vary as stimulation proceeds. For instance, while the timescale for long-term production is on the order of decades, a stimulation operation may take less than a day, and individual fractures may propagate via processes at the microsecond timescale. The spatial domain also varies drastically; reservoirs may be on the order of less than one to several miles, while a particular stimulation may only affect an area of several tens of feet from the action point. The choice of stimulation method also influences the time and spatial domains of resulting physical phenomena that must be considered. For instance, at short timescales and distances up to several tens of feet from detonation, the motion of the dynamic wave and the nonlinear response of the rock resulting from explosive stimulation will have a large impact on the structure and extent of fracturing very different from conventional hydrofracturing.

To capture faithfully the spatial/temporal domains required for simulation of reservoir behavior, a geomechanics simulation code must perform in a fashion similar to a set of video cameras with different lenses and the ability to speed up or slow down the frame rate as the situation requires. One camera can be kept on time-lapse mode to survey long-term, overall behavior. Once something is about to happen, another high-speed camera is started and zooms in on the area of interest (perhaps with a wavelength filter to see a different type of activity), and its feed is synchronized with that of the time-lapse camera. Together these provide a more complete view of a scene, eliminating the need to observe the entire scene at high spatial and temporal resolution. Simulations can be performed in a similar way by splitting operations over time and spatial scales and by applying different physical models at each of these scales. This type of adaptive scaling is an essential feature of the GEOS computational framework.

GEOS is a framework that will allow an analyst to couple different solvers in unique and sophisticated ways, adapted to various geologic settings, materials and stimulation methods. Currently, the GEOS development is focused on capturing the dominant processes during hydraulic stimulation of fracture networks in the subsurface. This problem is uniquely addressable with GEOS, which can run massively parallelized solvers (sequentially/concurrently) with different coupling interfaces. For most of the simulation, an implicit solver is employed at a coarse scale, allowing for fast computation of the evolution of the reservoir. When a fracturing event is imminent, the solver is transitioned to a more appropriate explicit solver that captures the time evolution of the event and then synchronizes with the implicit solver to continue its simulation.

Coupling between physics models occurs in a similar manner. For most of the time the hydraulic behavior of rock with pre-existing joints and fractures is governed by slow, convective, laminar flow through the porosity of the rock and narrow through-going channels and by even slower diffusive flow in the porous rock. However, during stimulation these time constants can be drastically reduced and non-laminar effects can dominate in the fractures where fracture propagation is occurring. The source mechanism of the fracture-associated seismic event will also be determined by GEOS and handed off to other wave propagation codes to predict the synthetic microseismicity at a particular site. Similarly, an asymmetric permeability tensor can be handed off to fluid and thermal transport codes. In the end, this scheme will provide a clear and consistent upscaling method to take the mechanisms that are observed at finer scales and homogenize them to larger scales for specific sites, providing the additional ability to capture uncertainty in the calculations as well as providing the basis for comprehensive risk analysis.

2. The Roadmap

The ***GEOS Initiative*** is a 3-year project funded by LLNL's Laboratory Directed Research and Development program (LDRD). Funding began in July, 2011 and will end in June, 2014. The primary purpose of this document is to assess the current state of GEOS code development and capabilities, and to outline development plans for the remainder of the initiative. There are some portions of the development plans that are mandatory and must be completed before the end of the project. Completion of these tasks will constitute ***GEOS 3.0***. Implementation of other features is somewhat more fluid and will depend upon the results of parametric testing and uncertainty quantification, applications to data from various stimulation activities along with input from potential sponsors regarding high-value targets (Figure 1). We will also describe some desired features that are unlikely to be considered during the remainder of the project, but remain as important targets for future consideration (Table 1). Timelines for the various program development activities is given in Figure 2.

2.1 Current state of *GEOS*

2.1.1 Status of Two dimensional implementation

The three dimensional implementation of GEOS is computationally intensive. A longer-term goal of the GEOS development effort, which likely will not be realized during the 3-year tenure of the project, is the development of derivative, fast-running, reduced complexity codes that can be traced back and verified using the full GEOS code. In the interim, we maintain a 2D modeling capabilities in GEOS that can be utilized in reconnaissance evaluation, and in uncertainty quantification and sensitivity analysis. The 2D implementation also provides a simpler visualization of the physical processes associated with stimulation. (NOTE: A longer-term goal of the GEOS development effort, is the development of derivative, fast-running, reduced complexity codes that can be traced back and verified using the full GEOS code – this will likely not be realized during the 3-year tenure of the project)

To date, the 2D implementation of GEOS runs in explicit mode incorporating:

1. First order triangular and quadrilateral finite elements.
2. Input and output (for visualization, user input, and restart capabilities) using the GEOS framework.
3. Fracturing and parallelization using the GEOS framework.

2.1.2 Status of Three dimensional implementation

The current three-dimensional implementation of GEOS is an explicit code, incorporating a parallel hydro-mechanical hexahedral/tetrahedral finite element linear elastic implementation with fracture (with cohesive elements) and arbitrary models of joint behavior.

We have:

1. Developed support for hydraulic fracture simulations by adding: (a) the ability to dynamically change the mesh topology (i.e., propagate a fracture along any face-constrained path), (b) suitable fracture criteria at the fine-scale (highly resolved crack tip) as well as the coarse-scale (under-resolved crack tip), and (c) special quasi-two-dimensional finite volume elements at separated faces (i.e., couple changes in fluid pressure with mechanical response) within the GEOS code framework for both the three-dimensional and massively parallel cases. This set of capabilities enables simulation of flow through the fracture network, as well as propagation of the network. Work has been completed for the explicitly integrated case, which is appropriate for dynamic loading rates; however, this will need to be revisited for inclusion of an implicit solver, which will provide support for the slower pressure propagation seen in many conventionally stimulated reservoirs. We have also implemented a model for a sub-fracture resolution of permeability (Barton-Bandis-Bakhter) alongside the LDEC model (Livermore Discrete Element Code) for joint dilation and normal response in the GEOS framework, enabling simulation of dilating, rough fractures. Verification of these models is ongoing.
2. Added a simple seismic source term generation model within the ***GEOS*** framework by incorporating an explicit, adjustable fidelity representation of the fractures in a Lagrangian framework. The current implementation has been demonstrated in simple problems, and the comparison of these preliminary results with field data has been promising.
3. Added capabilities to accommodate multiple, interacting fractures, which include the effects of induced stress fields in the near-field of the fracture process zone as well as the coalescence of fractures.
4. Developed quality assurance methodologies to reduce risk in the development process, including implementing an ATS-based test suite in the code as well as maintaining a version control system via a Subversion repository hosted on the TeamForge platform (maintained by LLNL).

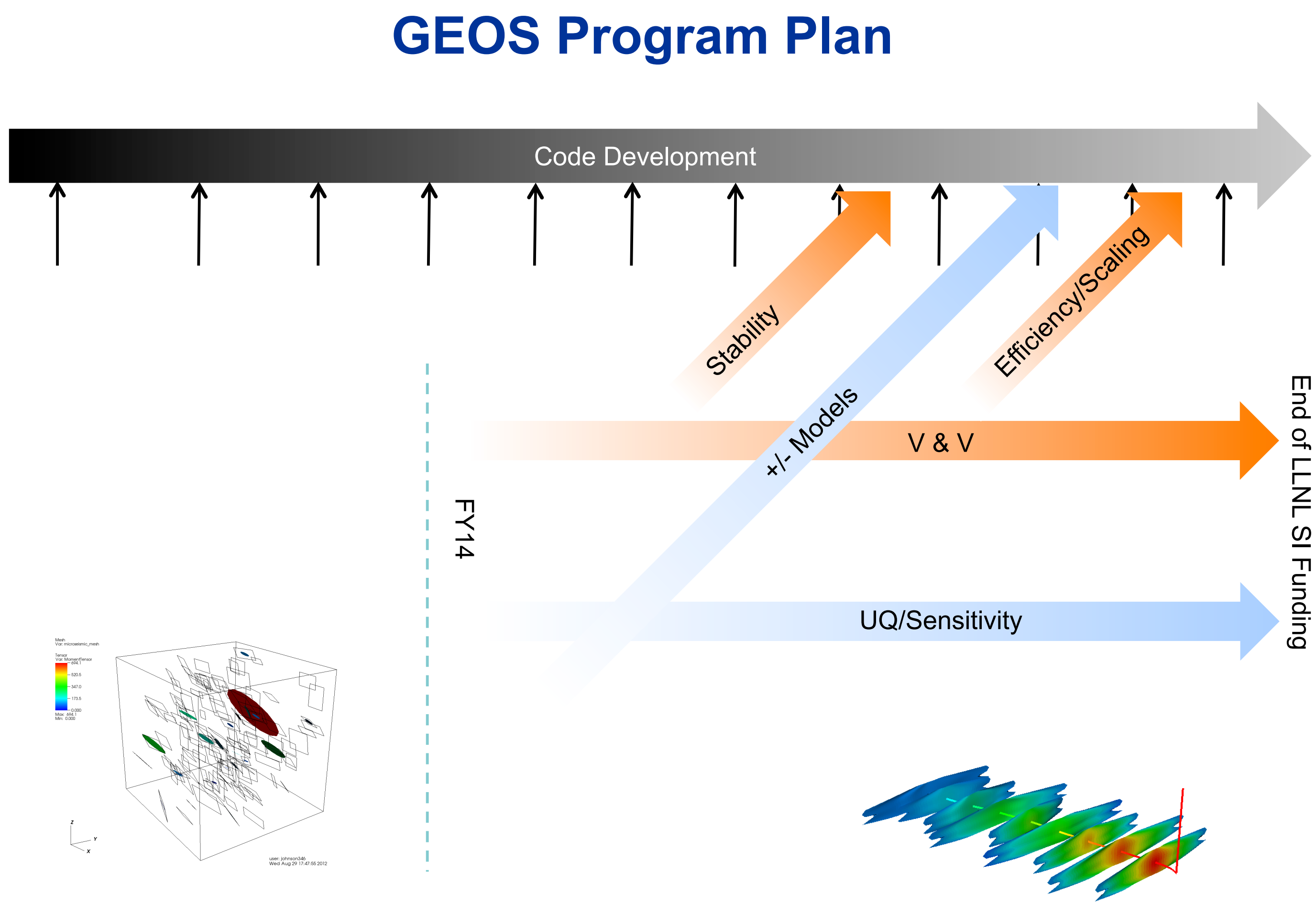

Figure 1. General plan for ***GEOS Strategic Initiative***. The first 2 years of the project were largely devoted to development of the GEOS code with links to LLNL seismic wave propagation codes, downscaling of LLNL “global” seismic tools for testing at reservoir scales and development of Uncertainty Quantification procedures with testing at 2D. The final year of the program will incorporate testing of the code against experimental and field data (V&V) and parametric testing and UQ of GEOS-3D. It is anticipated that such testing will result in code modification and perhaps the inclusion of additional physics models.

Table 1. Capabilities of GEOS 2D and 3D implementations

2D	3D
GEOS Computational Framework	GEOS Computational Framework
Triangular and quadrilateral finite elements.	Explicit Hydro-fracturing capability
Input and output (for visualization, user input, and restart capabilities	Simple seismic source term generation model within the ***GEOS*** framework
Fracturing and parallelization	Capabilities to accommodate multiple, interacting fractures
Parametric Testing - Uncertainty Quantification	Quality assurance methodologies to reduce risk in the development process
Implicit hydro-mechanics and fracture solvers	Implicit hydro-mechanics and fracture solvers
Coarse fracturing criterion	Coarse fracturing criterion
Enhanced material modeling framework	Enhanced material modeling framework
	Refined Sesimic Source modeling with coupling to wave propagation codes
	Multi-scale damage modeling for capturing seismo-hydro-mechanical behavior
	High strain rate fracturing - Deflagration-induced
	Parametric Testing - Uncertainty Quantification
	Coupling to Flow and Transport Codes
	High strain rate fracturing – Detonation-induced pressure pulse in fracture network
	High strain rate fracturing - Shock wave interaction induced tensile damage zones
	Node-splitting and remeshing
	Development of Fast-running, reduced complexity, derivative codes

Green – existing capabilities; Blue – capabilities under development, completion anticipated before the end of LLNL's Strategic Initiative; desired capabilities, not currently part of the GEOS Development Roadmap.

2.2 Future Developments

2.2.1 Implicit hydro-mechanics and fracture solvers

Perhaps the most important remaining issue in the overall development of the GEOS framework is implementation of the implicit hydro-mechanics and fracture solvers. In its current explicit mode the experimenter and issues concerning computational stability determine the simulation time-step, rather than the natural temporal scale of the physical processes involved. This results in computationally expensive simulations that are necessarily restricted to timeframes much shorter than those of field simulation. Implementation of this capability will constitute the beta version of ***GEOS 3.0***.

2.2.2 Coarse fracturing criterion – 2D and 3D implementations

The calculation of stress intensity factors (SIF) based on linear elastic fracture mechanics (LEFM) principles in massively parallel code is a challenging task. Because the ghost zone at domain partition boundaries only consists of one layer of elements, it is impractical to use the J-integral and its variants. Conventional displacement-based methods require special quarter-point finite elements in the first layer of elements around the fracture tip and substantial near-tip region mesh refinement. They are appropriate for simulations with known static fractures so that special meshing treatment can be undertaken in the pre-processing stage. We have developed a generalized form of the displacement correlation method (the GDC method), which can use any linear or quadratic finite element type with homogeneous meshing without local refinement. These two features are critical for modeling dynamic fracture propagation problems where locations of fractures are not known *a priori*. However, the GDC method cannot be implemented in the current version of GEOS because it requires information in two layers of elements around the fracture tip if linear elements are used or one layer for quadratic elements. The first scenario is ruled out by the thickness of the ghost zone at domain partition boundaries. The second scenario is precluded by the currently available element types, and the implementation of quadratic elements is not included in the current roadmap.

We will implement an alternative method for the calculation of SIF, called the Virtual Crack Closure Technique (VCCT). This method works for both 2D and 3D elements and only requires one layer of elements around a tip. The main disadvantage of VCCT compared with the GDC method is that it cannot handle the scenarios of fracture initiation from kinks and propagating fractures crossing existing fractures. These will be mitigated by randomly placing small fissures along existing fractures to allow hydraulic fractures to initiate from the tips of these fissures. This treatment is supported by field observations reported in the literature.

VCCT will first be implemented in 2D. A significant problem in 3D not seen in 2D is that the fracture geometry is difficult to resolve. Instead of the front being a single node or edge, the front becomes either an arbitrary set of edges or an arbitrary surface.

Similarly, the geometry behind the front goes from a 2D set of easily determined edges to an arbitrary surface, which may or may not be closed. These are both significant computational geometry challenges. We will determine the feasibility and issues involved in extending VCCT (or creating an alternate method) for use in 3D simulations.

2.2.3 Material modeling framework

GEOS operates on geologic models that describe materials properties, pre-existing fracture networks within the reservoir, etc. The activities described here are designed to optimize and enhance the coupling of materials models and the GEOS code.

1. Port vectorized representation to packet-based representation.
2. Design and implement consistent interfaces.
3. Implement 3D table-based state initialization.
4. Implement stochastic description of initial states.
5. Implement analytical description of initial states.
6. Inclusion of the GEODYN material library.

2.2.4 Seismic source modeling

Fracturing during hydraulic stimulation is most directly and immediately observed by the microseismic response. GEOS will simulate the time history of hydraulically induced fracture, and comparison with observed seismicity requires that GEOS generate a source term and then pass that to a seismic wave propagation code to produce synthetic seismograms for surface and borehole seismic arrays. This is one of the initiatives primary deliverables and will be accomplished during the final year of the project. One of the complications is that the magnitudes of observed seismic events suggest that the amount of slip is small relative to the grid spacing used in typical simulations. Resolving these features a sub-grid scale represents one of the challenges in GEOS development. Necessary activities include:

1. Implement infrastructure. This will be dependent on overhaul of material modeling implementation.
2. One-way coupling: mechanical to source using a sub-scale, Geostatistically defined representation of heterogeneity.
3. Two-way coupling: mechanical-damage. Working with Chloe Arson (Georgia Institute of Technology) plan developed (March 2013) and is detailed in the following sub-section.
4. Three-way coupling: mechanical-damage-permeability. Working with Chloe Arson, including work from other group members and literature for coupled permeability-mechanical joint models; details are included in the following sub-section
5. Coupling with WPP: Implemented output from GEOS that can be directly read by LLNL seismic wave propagation codes, WPP/SW4.

6. Multi-scale refinement: A dual-scale paradigm for sequential, hierarchical multi-scale treatment of the coupled hydro-mechanical problem is being pursued as part of the work with Georgia Tech and is detailed in the following sub-section.

2.2.5 Multi-scale damage modeling for capturing seismo-hydro-mechanical behavior

One key component of the modeling strategy is to be able to capture contributions to the behavior of the reservoir that occur at scales below that explicitly represented in the simulation (sub-RVE). That is, we need a method of upscaling fine scale effects to coarser scales. To achieve this, we are currently pursuing a sequential, hierarchical multi-scale approach based on thermodynamically consistent, stochastic methods for representing coupled damage processes in brittle materials.

Specifically, we will be using Continuum Damage Mechanics (CDM) to predict the statistical average response of cracked solids, without describing the real geometry of each micro-crack, which is necessary in order to reduce the number of degrees-of-freedom in the problem to a computationally tractable size given that the memory and processing capacities of the HPC resources are already anticipated to be limiting for the applications of interest. This theoretical framework was initially designed to model the brittle behavior of metals but has applications to damage of brittle geomaterials. In micro-mechanical damage models, the main challenge consists of characterizing the set of cracks present in the medium according to their size and orientation. Within each set, crack growth is generally controlled by a Griffith criterion. The natural dissipation variable should be the length of the cracks within the set considered, but crack densities are generally preferred. For each crack set, the thermodynamic variable conjugate to crack density is referred to as the "affinity" or "damage force". The Griffith criterion is met when the derivative of the affinity to crack density is more than a certain critical value. If the threshold is reached, crack densities must be updated. The damaged stiffness tensor can then be constructed by accounting for the updated crack geometry in an appropriate homogenization scheme (e.g. the self-consistent method or Mori-Tanaka scheme).

In general terms, the steps necessary to implement this will be:

1. Determine constitutive relationships to predict microscopic crack initiation and propagation.
    a. Characterize the microstructure parameters and their conjugate affinities.
    b. Relate affinities to stress and microstructure parameters to texture-related functions.
2. Determine the functional dependence of RVE size on microstructural properties.

3. Determine appropriate coupling terms to achieve equivalence between continuum (stochastic) and discrete representations.
4. Determine thresholds at which to advect microstructural damage into explicitly represented fracture surfaces.

Many parts of this approach are well-defined; however, despite some research, the connection between microstructural parameters and their conjugate affinities will be an area that requires additional research to properly address. In general, the completion timeline for the multi-scale approach will be difficult to forecast until we have more maturity in our work in the area, but we have secured funding to bring in both Dr. Arson as well as a student for the summer of 2013 in order to expedite these advances.

2.2.6 Uncertainty Quantification (UQ)

Evaluating the uncertainty is an essential element of parametric testing of GEOS, and its application to forward predictions of reservoir stimulation. Also, by constraining the sensitivity of various predictions to variations in reservoir and operational variables, UQ constitutes an important precursory step to the development of derivative, reduced complexity, fast running tools. Along with operational parameters, there are a variety of uncertainties associated with the geologic model including the nature of pre-existing fracture distributions and rock mechanical properties which require evaluation if optimization is to be achieved. Here we will link GEOS with the LLNL UQ code, PSUADE (**P**roblem **S**olving environment for **U**ncertainty quantification **A**nd **D**esign **E**xploration) which is a suite of uncertainty quantification modules capable of addressing high-dimensional sampling, parameter screening, global sensitivity analysis, response surface analysis, uncertainty assessment, numerical calibration, and optimization. This linkage has already been successfully implemented with an earlier 2D version of the GEOS capabilities, resulting in the establishment of sensitivity curves for a number of process and geologic parameters.

2.2.7 High strain rate fracturing

While much of our current effort is directed at optimization of the hydraulic stimulation, we recognize the need for a computational tool to aid in the design of new stimulation methods that minimize water use and potentially involve the use of energetic materials. Current personnel and time constraints may preclude significant advances in these areas during the current project. Here we describe the requirements for three separate scenarios utilizing energetic stimulation. In the simplest case, we could use the current infrastructure with a special time-dependent joint model to capture the behavior. In the ideal case, full coupling of GEOS with GEODYN, a parallel transient Eulerian finite volume code with constitutive models that are well suited for analyzing the dynamic response of geologic media, would be undertaken. Use cases include:

2.2.7.1 Deflagration-induced pressure elevation in fracture network

If this is the case, and we do not need to consider the propagation of the shockwave associated with detonation, but rather the introduction of a source term to produce the higher pressures. This is relatively straightforward within the existing GEOS framework, and will be accomplished during the Initiative.

2.2.7.2 Detonation-induced pressure pulse in fracture network

Simulation of this scenario, would require modification of our basic hydrofracture capability to enable:

1. Transmission of waves through the fluid.
2. Production of the actual shock.

The confined nature of this problem may or may not lend itself to a simple quasi-two-dimensional empirical approach that takes advantage of the parallel plate geometry of a fracture. This application will at least be explored during the current project.

2.2.7.3 Shock wave interaction induced tensile damage zones

This type of simulation requires strong coupling between GEOS and GEODYN. A fully coupled 3D GEOS/GEODYN code requires passing the fracture geometry to GEODYN which then interprets the geometry and constructs volume fractions on its internal regular grid representation, performs its calculations, then passes back vector forces for each face it was given. Another complication is that not only is re-gridding required but also information on the parallel partitioning of GEOS must be parceled out (efficiently) to the spatial partitions in GEODYN that require the information. We have addressed this with the Bifroest framework. Accomplishing this along with evaluation of alternative approaches (use GEODYN as an initializer to a Lagrangian code rather than a fully coupled simulation) would likely require at least 2 years of effort. In the interim, aspects of energetic material detonation can be explored using the existing version of GEODYN.

2.2.8 Framework for fluid flow models

GEOS will provide a permeability tensor for a given geologic model and stimulation scenario. The spatial distribution of permeability can then be used as a starting point for other fluid, thermal and proppant transport models. Some of the features of these models will be simulated in GEOS, but full coupling is not likely to be computationally feasible at this time. For instance, the long-term evolution of an enhanced geothermal reservoir would necessarily require consideration of fluid-rock interaction, which is beyond the scope of the current investigation. However, efficient linking of GEOS predictions with such models, as in the case of coupling GEOS and seismic wave propagation codes is desirable. A specific example is linking GEOS output files to the LLNL flow and transport code, NUFT.

NUFT-C (Non-isothermal, Unsaturated Flow and Transport with Chemistry) is a code designed to simulate coupled fluid movement (multiple liquids and gas) and chemical reactions in saturated or unsaturated porous media. Chemical interactions that modify the physical properties of the porous media are also considered. Applications of the code have primarily addressed simulations of the long-term evolution of rock in the vicinity of deep geological high-level nuclear waste repositories, thermal perturbation of sedimentary basins, and mineral and chemical evolution associated with subsurface sequestration of CO_2. GEOS can provide the base model upon which NUFT and other codes can operate.

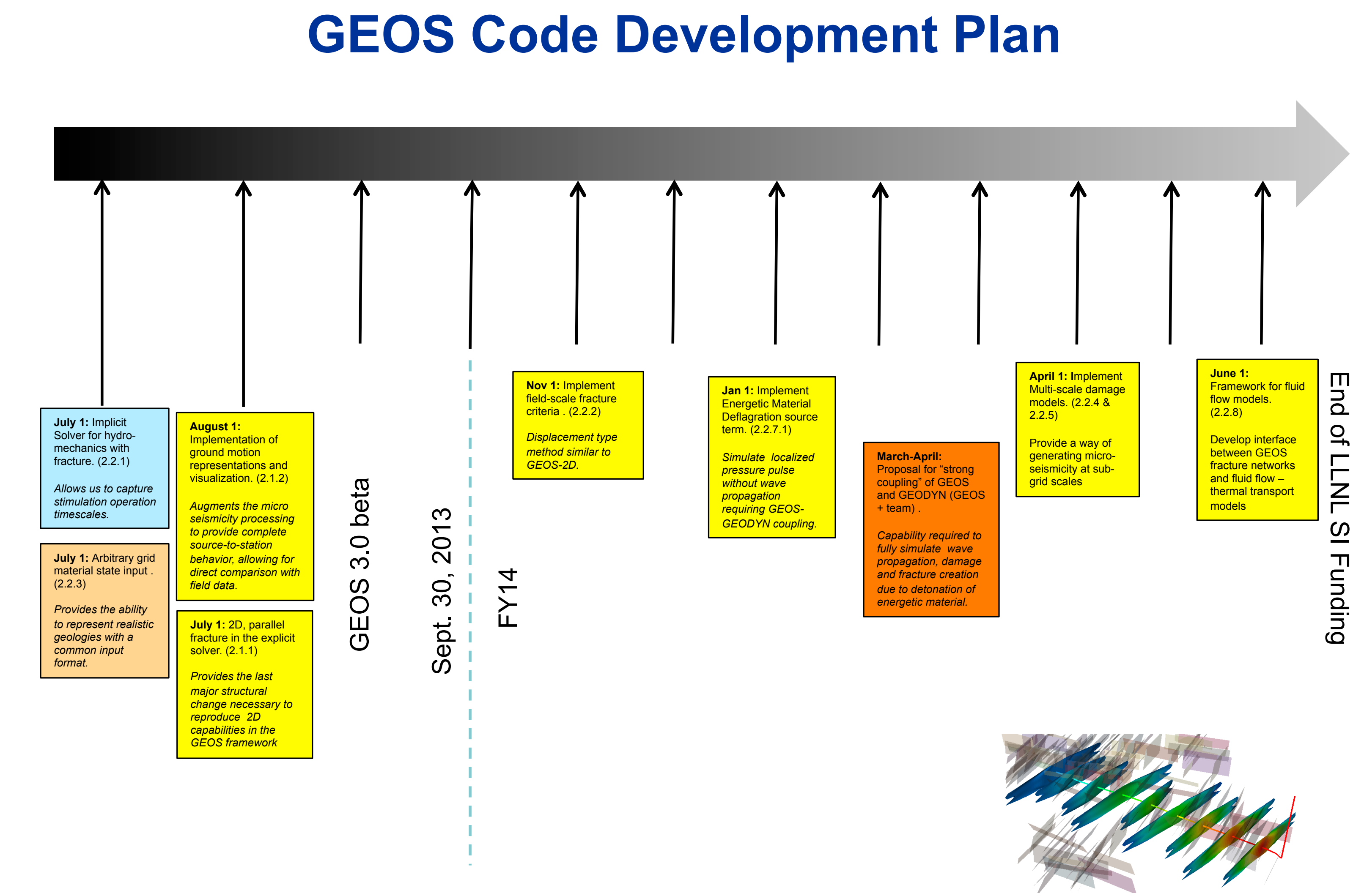

Figure 2. ***GEOS*** Code Development Roadmap. Presented here are the current code development milestones with approximate dates. The milestones are also keyed to the text. The critical elements are those occurring before the end of FY13 – Sept. 30, 2014 and will constitute the beta version of ***GEOS 3.0***.